CHEMICAL PHYSICS

Volume 184, number 1,2,3, 15 June 1994

Contents

The vibrational and temperature dependence of the magnetic properties of the oxonium ion (H_3O^+)	
S.P.A. Sauer, V. Špirko, I. Paidarová and J. Oddershede	1
Electron momentum distributions and ionization energy spectra of boron trifluoride E. Weigold, Y. Zheng and W. von Niessen	13
An intermolecular potential for $(O_2)_2$ involving $O_2(^1\Delta_g)$ B. Bussery	29
Sequential and superexchange electron-transfer reactions in a three-component system J. Tang	39
Formation of NH ⁺ ₄ at the Brønsted site in SAPO catalysts J. Limtrakul and J. Yoinuan	51
A theoretical description of the ion BeC ⁺ and the photoelectron spectrum of BeC A.C. Borin and F.R. Ornellas	59
Quantum chemical investigation of the Ar-HCl interaction potential. Steepness and asymmetry with implications for energy transfer M. Simonson, T.D. Sewell, S. Nordholm and A. Miklavc	67
Theoretical study of the mono- and di-hydrated divalent ions of the first-row transition metals R. Åkesson and L.G.M. Petterson	85
Potential energy surfaces of some low-lying states of fluoroformyl radical FCO S. Nanbu, M. Gomyo and S. Iwata	97
Theoretical study of spectroscopic properties of cubane V. Galasso	107
Theoretical investigation of potential energy surfaces relevant for excited-state hydrogen transfer in o-hydroxybenzaldehyde	
A.L. Sobolewski and W. Domcke On the evolution of cluster to bulk properties: a theoretical LCGTO-LDF study of free and	115
coordinated Ni _n clusters (n=6-147) G. Pacchioni, SC. Chung, S. Krüger and N. Rösch	125
π-electron force field in internal coordinates for trans- and cis-polyacetylene A. Girlando, A. Painelli, G.W. Hayden and Z.G. Soos	139
Spectroscopic and theoretical studies on a three-iron cluster with linear arrangement H. Paulsen, XQ. Ding, M. Grodzicki, Ch. Butzlaff, A.X. Trautwein, R. Hartung and	
K. Wieghardt	149

(continued on page 3 of cover)



0301-0104(19940615)184:1/3;1-K

Contents

(continued from page 4 of cover)

A smooth truncation for polarizable water B.J. Palmer	163
The theory of the diffusion-controlled reaction $A+B\rightarrow 0$ with arbitrary concentrations of reagents M.G. Golubkov, A.S. Prostnev and B.R. Shub	171
on-molecule processes in the interstellar medium. Rates for rotational excitations in NH ₃ -H ⁺ collisions F.A. Gianturco and F. Ragnetti	177
A generalized Langevin equation for wave functions. Intramolecular vibrational dephasing as a stochastic process K. Someda and R.D. Levine	187
Differential photoionization cross section calculations for H ₂ S using the random phase approximation with L ² basis functions I. Cacelli, V. Carravetta and R. Moccia	213
A far infrared study of benzene-fluorinated benzene binary mixtures T. Tassaing, Y. Danten, M. Besnard, E. Zoïdis and J. Yarwood	225
Tentative identification of C_5N_2 in rare gas matrices A.M. Smith, C. Engel, A. Thoma, G. Schallmoser, B.E. Wurfel and V.E. Bondybey	233
Exciton-phonon coupling and pressure-induced structural phase changes in coronene crystals T. Yamamoto, S. Nakatani, T. Nakamura, K. Mizuno, A.H. Matsui, Y. Akahama and H. Kawamura	247
Excited states of azo compounds. II. Vibrational structure of the electronic absorption spectra of 4,4'-di-substituted azobenzene derivatives S. Luňák Jr., M. Nepraš, R. Hrdina and H. Mustroph	255
Dual phosphorescence from 2-(2'-hydroxyphenyl)benzoxazole in amorphous solid solution. Temperature dependence of dispersive kinetics of nonexponential triplet decay B. Nickel and A.A. Ruth	261
Excitation transfer for Xe* $(^{3}P_{2}) + N_{2}$ in the eV energy range: double potential crossing for N ₂ (B, $\nu'=5$) T.G. Aardema, E.J. van Nijnatten and H.C.W. Beijerinck	273
New model of charge carrier photogeneration for poly (N-vinylcarbazole) V. Cimrová and S. Nešpůrek	283
Valence-shell electronic structures of cis- and trans-butene: ionic-state-resolved orientationally averaged electron momentum densities by symmetric noncoplanar (e, 2e) spectroscopy C.P. Mathers, J.F. Ying, B.N. Gover and K.T. Leung	295
Charge-transfer production of predissociated N_2 states. I. The $n=3$ Rydberg state region (12.8–14 eV) A.B. van der Kamp, P.C. Cosby and W.J. van der Zande	319
Kinetics of multiphoton excitation and fragmentation of C_{60} P. Wurz and K.R. Lykke	335

(continued on preceding page)

Contents

(continued from page 3 of cover)

Spectral hole-burning and Stark effect: frequency dependence of the induced dipole moment of a squaraine dye in polymers E. Vauthey, J. Voss, C. de Caro, A. Renn and U.P. Wild	347
Resonant two-photon ionization detection of atomic iodine resulting from photodissociation of allyl iodide under vibrational (C-H overtone) excitation	347
A.V. Baklanov, V.P. Maltsev, L. Karlsson, B. Lindgren and U. Sassenberg	357
Positronium solvation sites in liquid amides revealed by magnetic field effects: influence of the chemical structure of the molecules I. Billard, J.Ch. Abbé and G. Duplâtre	365
Characteristics of a positronium bound state with nitrobenzene in methanol as deduced from magnetic field effects at various temperatures	271
G. Duplâtre, I. Billard and J.Ch. Abbé	371
Author index	378
Subject index	382
Instructions to authors	392